Claims

1-17 (Cancelled).

18. (Currently Amended)

A method for identifying a molecular interaction network of interacting molecules for a set of molecules within a biological system, wherein said interacting molecules have one or more conserved features, said method comprising:

determining attraction probabilities between said conserved features of different molecules within the set of molecules based on known molecular interaction networks;

determining a single network probability of each possible network based on a molecular interaction probability of each pair of the reacting molecules within said each network, wherein said molecular interaction probability is determined by using the attraction probabilities between features of the interacting molecules;

determining a sampling probability of said each network based on network topology of said each network;

determining a network probability of each network as a product of said single network probability and said sampling probability; and

identifying the network having the highest network probability as the molecular interaction network of interacting molecules for the set of molecules.

Computer readable medium for identifying a most likely biological pathway of a set of interacting molecules, wherein said interacting molecules each have one or more conserved features, the computer readable medium comprising instructions operable to perform the steps of:

- a. representing the set of interacting molecules as oriented network graph, G = <V, E>, where the vertices, V, correspond to molecules, and the edges or connections E, correspond to interactions between molecules;
- b. <u>assigning a probability P(network) to each possible oriented network graph</u> found from a fixed number of vertices V; and
- c. selecting an oriented network graph as the most likely biological pathway based on the probabilities P(network) assigned to all possible oriented network graphs, whereby the selected graph provides a molecular interaction network representation of the biological pathway,

wherein step (b) comprises:

- (i) assigning an attraction probability p_{ij} to every pair of molecules i and j that the molecules are connected to each other by an oriented edge, and conversely a probability (1-p_{ij}) that the molecules are not connected to each other by an oriented edge;
- (ii) computing a probability P(E) that a network has a particular edge set E (ε_{ii}):
- (iii) sorting all the possible oriented network graphs into a finite number of bins, each corresponding to a particular network topology that corresponds to a particular distribution of edges coming into and out of each vertex in the particular network, so that each bin represents a collection of oriented network graphs characterized by the same network topology;
 - (iv) computing a probability P(topology) for each bin; and
 - (v) computing P(network) as the product of P(E) and P(topology).
- 19. (Currently Amended) The <u>computer readable medium method</u> of claim 17 18, wherein said attraction probabilities <u>p</u>_{ij} are dependent on the conserved features of each molecule and are <u>between said conserved features</u> are determined by

quantifying the occurrence frequency of said features at immediately upstream or downstream of each other within the known networks.

- 20. (Cancelled)
- 21. (Currently Amended) The <u>computer readable medium method</u> of claim 17 18, wherein said attraction probabilities <u>pij</u> of said features are determined by using equation 14. by quantifying the number of times conserved features in every pair of molecules i and j are seen in interaction with each other in known networks.
- 22. (Cancelled).
- 23. (Cancelled).
- 24. (Cancelled)
- 25. (Currently Amended) The <u>computer readable medium method</u> of claim 17 18, further comprising <u>instructions operable to perform the step of obtaining a posterior probability of each <u>possible oriented network graph</u>, and wherein said selected <u>oriented molecular interaction</u> network <u>graph corresponds to the graph having the highest network probability is the network having the highest posterior probability.</u></u>
- 26. (Currently Amended) The <u>computer readable medium method</u> of claim 24 25, wherein said posterior probability is determined by using Markov Chain Monte Carlo techniques.
- 27. (Currently Amended) The <u>computer readable medium method</u> of claim 17 18, wherein said interacting molecules are proteins and said conserved features are protein domains or motifs.
- 28. (Currently Amended) The <u>computer readable medium</u> method of claim 26 27, wherein said conserved features are nucleic acid motifs.
- 29. (Currently Amended) The <u>computer readable medium</u> method of claim 26 27, wherein said <u>attraction</u> probabilities <u>p</u>_{ij} between said conserved features are

determined by quantifying the occurrence frequency of said <u>conserved</u> features at immediately upstream or downstream <u>of</u> each other within the known networks; and said <u>molecular interaction probability attraction</u> probability <u>pij</u> of each pair of reaction molecules is determined by <u>quantifying the number of times conserved</u> features in every pair of molecules i and j are seen in interaction with each other in <u>the known networks using equation 6 or 14</u>.

30. (Cancelled)

- 31. (Currently Amended) The <u>computer readable medium method</u> of claim 26 27, wherein said topology-probability P(topology) of each possible network is a product of incoming edge distribution probability and outgoing edge distribution probability within said each possible network; and further comprising step of obtaining posterior probability of each network, wherein said molecular interaction network having the highest network probability is the network having the highest posterior probability, wherein said highest posterior probability is determined by Markov Chain Monte Carlo techniques.
- 32. (Currently Amended) The <u>computer readable medium</u> method of claim 30 31, wherein said attraction probabilities of said features are determined by <u>quantifying</u> the number of times conserved features in every pair of molecules i and j are seen in interaction with each other within the known networks using equation 6 or 14.
- 33. (Currently Amended) The <u>computer readable medium</u> method of claim 30 31, wherein said attraction probabilities of said features are determined by <u>quantifying</u> the number of times conserved features in every pair of molecules i and j are seen in interaction with each other within the known networks using equation 14.
- 34. (Cancelled)
- 35. (Cancelled)
- 36. (Currently Amended) A <u>computer readable medium method</u> for identifying a molecular interaction network <u>representation</u> of interacting molecules for a set of

interacting molecules within a known biological system, wherein <u>each of</u> said interacting molecules have one or more conserved features, <u>said method</u> the <u>computer readable medium</u> comprising <u>instructions operable to perform the steps</u> of:

- a. determining attraction probabilities between said conserved features of pairs of different molecules of the set of interacting molecules based on known molecular interaction data where in said attraction probabilities are determined by quantifying the occurrence frequency of said conserved features of said pair of molecules at immediately upstream or downstream of each other within the known biological system networks and using equation 6 or 14;
- b. determining a single network an edge probability P(E) for of each possible molecular interaction network of the set of interacting molecules, based on molecular interaction the determined attraction probabilities of each pair of interacting reaction—molecules within said each possible molecular interaction network using equation 5 or 17;
- c. determining a sampling topology probability <u>P(topology)</u> of said each <u>possible molecular interaction</u> network based on the network topology of said <u>each</u> network, said <u>sampling topology</u> probability being a product of <u>an</u> incoming edge distribution probability and <u>an</u> outgoing edge distribution probability within said each possible <u>molecular interaction</u> network.
- d. determining a network probability of <u>said</u> each <u>possible molecular</u> interaction network as a product of said <u>single network edge</u> probability <u>P(E)</u> and said topology probability <u>P(topology)</u>;
- e. determining a posterior probability of said each <u>possible molecular</u> interaction network using equation 10; and

- f. identifying the <u>possible molecular interaction</u> network having the highest posterior probability as said molecular interaction network <u>representation</u> of interacting molecules for the set of <u>interacting</u> molecules.
- 37. (Currently Amended) The <u>computer readable medium</u> method of claim 35 36, wherein said molecule[s] is a are protein and said conserved features are protein domain or motif.
- 38. (Currently Amended) A <u>computer readable medium method</u> for identifying a molecular interaction of a molecule within a biological network wherein said biological network comprises a set of interacting molecules, and said interacting molecules have each having one or more conserved features, said method the computer readable medium comprising instructions operable to perform the steps of:
 - a. identifying a conserved feature of said molecule
 - determining attraction probabilities between the conserved features of said molecule and the <u>other</u> interacting molecules based on known molecular interaction data of the biological network;
 - c. determining molecular <u>interaction</u> probabilities of said molecule with each of the <u>other</u> interacting molecules based on the attraction probabilities; and
 - d. identifying the molecular interaction of said molecule with a <u>one of the other</u> interacting molecules, which provides highest molecular probability with said molecule corresponding to the highest of the determined molecular interaction probabilities.
- 39. (Currently Amended) The <u>computer readable medium method</u> of claim 37 38, wherein said attraction probabilities of said features are determined by using equation 6 or 14.

- 40. (Currently Amended) The <u>computer readable medium</u> method of claim 37 38, wherein said attraction probabilities of said features are determined by using equation 14.
- 41. (Currently Amended) The <u>computer readable medium method</u> of claim 37 38, wherein said molecular probability of the molecular interaction between said two molecules is identified by using equations 5 or 17.
- 42. (Currently Amended) The <u>computer readable medium</u> method of claim 37 38, wherein said likelihood of molecular interactions between said interacting molecules is determined by using equations 17.
- 43. (Currently Amended) The <u>computer readable medium method</u> of claim 37 38, wherein said molecules are protein, and said conserved features are protein domain or motif.
- 44. (Currently Amended) A screening method for identification of a compound capable of modifying the interaction between at least two molecules with in a biology network comprising
 - a. identifying an interaction between said at least two molecules using the method of claim 37 38;
 - b. introducing a test compound in the biology network, the test compound contacting said at least two molecules said proteins identified in step (a) with a test compound;
 - c. comparing the <u>identified</u> interaction of the molecules in the presence of the test compound with the <u>identified</u> interaction in the absence of the test compound;

wherein a difference in the <u>identified</u> interaction of the molecules in the presence of the test compound as compared to the interaction in the absence of a test compound indicates identification of a compound capable of modifying the interaction between molecules.

45. (Currently Amended) The screening method of claim 43 44, wherein said molecules are proteins.